FTML Project

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1 Bayes estimator and Bayes risk

Question 1

- Input space $\mathcal{X} = [0; 1]$
- Output space $\mathcal{Y} = \mathbb{R}^+$
- X uniform continuous distribution on $\mathcal{X}$
- $l(x, y) =$ squared loss
- Y $\sim$ Exp(1 + X)

The Bayes estimator in respect to the squared loss is $f^*(x) = E[Y|X = x]$, so

$$f^*(x) = E[Y \sim Exp(1 + x)]$$

We know that $E[X \sim Exp(\lambda)] = \frac{1}{\lambda}$ so

$$\mathbf{f^*(x) = \frac{1}{1 + x}}$$

And the Bayes Risk is

$$R^* = E[l(Y, f^*(X))]$$
$$= E_X[E_Y[(Y - f^*(X))^2|X]]$$
$$= E_X[Var(Y|X)]$$

We know that $Var[X \sim Exp(\lambda)] = \frac{1}{\lambda^2}$

$$= E_X[\frac{1}{(1 + X)^2}]$$
$$= \int_0^1 \frac{1}{(1 + x)^2} dx = \left[-\frac{1}{1 + x}\right]_0^1$$
$$= \mathbf{\frac{1}{2}}$$

Question 2

Let's define $\tilde{f}$ as the OLS estimator, which means

$$\tilde{f} = \begin{cases} \mathcal{X} \to \mathcal{Y} \\ x \to \hat{\theta}_1 x + \hat{\theta}_2 \end{cases}$$

With $\hat{\theta}_1$ and $\hat{\theta}_2$ the scalar parameters that minimize the squared loss. We deduce that

$$\begin{aligned}
\hat{\theta}_1 &= \frac{Cov(X,Y)}{Var(X)} \\
&= 12 * Cov(X,Y) \\
&= 12\left(E[XY] - E[X]E[Y]\right) \\
&= 12\left(E[E[XY|X]] - E[X]E[E[Y|X]]\right) \\
&= 12\left(E[\mathbf{XE[Y|X]}] - E[X]E[E[Y|X]]\right) \\
&= 12\left(E[\frac{X}{1+X}] - E[X]E[\frac{1}{1+X}]\right) \\
&= 12\left(1 - log(2) - \frac{1}{2}log(2)\right) \\
&= \mathbf{12 - 13log(2)}
\end{aligned}$$

And

$$\begin{aligned}
\hat{\theta}_2 &= E[Y] - \hat{\theta}_1 E[X] \\
&= E[E[Y|X]] - \hat{\theta}_1 \frac{1}{2} \\
&= log(2) - \frac{1}{2}(12 - 13log(2)) \\
&= \mathbf{\frac{15}{2}log(2) - 6}
\end{aligned}$$

We conclude that

$$\tilde{f}(x) = (12 - 13log(2))x + \frac{15}{2}log(2) - 6$$

The simulation in `part1_simulation.py` with the above settings and 10 000 samples of (X,Y) suggests that the Bayes estimator is better at estimating the setting than the OLS estimator. Probably because our model is not linear. Furthermore, the computed generalization error of the Bayes estimator converges to the value of the Bayes Risk we found previously ($\sim 1/2$) which lets us think that the simulation is a good estimation of the theoretical setup.

2 Bayes risk with absolute loss

Question 1

P(Y|X=x) where P corresponds to an Exp(λ) continuous distribution.
The Bayes estimator for l_2 squared loss

$$f_2^*(x) = E[Y|X = x] = E[\lambda e^{-\lambda}] = \frac{1}{\lambda}$$

The Bayes estimator for l_1 absolute loss is the median of Y|X=x as seen in Question 2

$$f_1^*(x) = \frac{ln(2)}{\lambda}$$

These Bayes estimators are not equal.

Question 2

We note $p = p_{Y|X=x}$

$$g(z) = \int_{\mathbb{R}} |y - z| p(y) dy$$

$$= \int_z^{+\infty} (y - z) p(y) dy + \int_{-\infty}^{z} (z - y) p(y) dy$$

$$= \int_z^{+\infty} yp(y) dy - z \int_z^{+\infty} p(y) dy + z \int_{-\infty}^{z} p(y) dy - \int_{-\infty}^{z} yp(y) dy$$

$$\frac{d}{dz} g(z) = -zp(z) - \left(\int_z^{+\infty} p(y) dy - zp(z) \right) + \left(\int_{-\infty}^{z} p(y) dy + zp(z) \right) - zp(z)$$

$$= \int_{-\infty}^{z} p(y) dy - \int_z^{+\infty} p(y) dy$$

Thus, $\frac{d}{dz} g(z) = 0$ if :

$$\int_{-\infty}^{z} p(y) dy = \int_z^{+\infty} p(y) dy$$

This occurs when both sides are equal to $\frac{1}{2}$, which means that the Bayes estimator $f^*(x)$ is the median. But to confirm this minimizes g(z), let's check the second derivative:

$$\frac{d^2}{dz^2} g(z) = 2p(z) > 0$$

The second derivative is always positive, so our solution is a minimum.

3 Expected value of empirical risk

Exercise

Step 1 :

$$E\left[R_n(\hat{\theta})\right] = E\left[\frac{1}{n}||y - X\hat{\theta}||_2^2\right]$$

$$= E\left[\frac{1}{n}||y - X((X^TX)^{-1}X^Ty)||_2^2\right]$$

$$= E\left[\frac{1}{n}||(I_n - X(X^TX)^{-1}X^T)y||_2^2\right]$$

$$= E\left[\frac{1}{n}||(I_n - X(X^TX)^{-1}X^T)(X\theta^* + \epsilon)||_2^2\right]$$

$$= E\left[\frac{1}{n}||X\theta^* + \epsilon - X\underbrace{(\mathbf{X^TX})^{-1}\mathbf{X^TX}}_{=\mathbf{I_d}}\theta^* - (X(X^TX)^{-1}X^T)\epsilon||_2^2\right]$$

$$= E\left[\frac{1}{n}||X\theta^* + \epsilon - X\theta^* - (X(X^TX)^{-1}X^T)\epsilon||_2^2\right]$$

$$= E\left[\frac{1}{n}||\epsilon - (X(X^TX)^{-1}X^T)\epsilon||_2^2\right]$$

$$= E_\epsilon\left[\frac{1}{n}||(I_n - X(X^TX)^{-1}X^T)\epsilon||_2^2\right]$$

Step 2 :

$$A \in \mathbb{R}^{n,m} B \in \mathbb{R}^{n,m}$$

$$tr(A^TB) = \sum_{i,j \in [1,n]\times[1,m]} a_{ij}b_{ij}$$

Thus :

$$A \in \mathbb{R}^{n,n}$$

$$tr(A^TA) = \sum_{i,j} a_{ij}a_{ij}$$

Step 3 :

$$E_\epsilon\left[\frac{1}{n}||A\epsilon||^2\right] = E_\epsilon\left[\frac{1}{n}\sum_{i=1}^{n}(A\epsilon)_i^2\right]$$

$$= E_\epsilon\left[\frac{1}{n}tr((A\epsilon)^T(A\epsilon))\right]$$

$$= E_\epsilon\left[\frac{1}{n}tr(\epsilon^T A^T A\epsilon)\right]$$

The trace is invariant under cyclic permutation.

$$= E_\epsilon\left[\frac{1}{n}tr(\epsilon\epsilon^T A^T A)\right]$$

By linearity of the trace and the expected value, we can push the expectation inside.

$$= \frac{1}{n}tr(E_\epsilon[\epsilon\epsilon^T]A^T A)$$

$$= \frac{1}{n}tr(\sigma^2 I_n A^T A)$$

$$= \frac{1}{n}tr(A^T A)\sigma^2$$

Step 4 :

$$A = I_n - X(X^T X)^{-1}X^T$$

$$A^T A = (I_n - X(X^T X)^{-1}X^T)^T(I_n - X(X^T X)^{-1}X^T)$$

$$= (\mathbf{I_n^T} - (\mathbf{X}(\mathbf{X^T X})^{-\mathbf{1}}\mathbf{X^T})^{\mathbf{T}})(I_n - X(X^T X)^{-1}X^T)$$

$$= (\mathbf{I_n} - (\mathbf{X^T})^{\mathbf{T}}((\mathbf{X^T X})^{-\mathbf{1}})^{\mathbf{T}}\mathbf{X^T})(I_n - X(X^T X)^{-1}X^T)$$

$$= (\mathbf{I_n} - \mathbf{X}(\mathbf{X^T X})^{-\mathbf{1}}\mathbf{X^T})(I_n - X(X^T X)^{-1}X^T)$$

$$= (I_n - X(X^T X)^{-1}X^T)^2$$

$$= I_n - 2X(X^T X)^{-1}X^T + (X(X^T X)^{-1}X^T)^2$$

$$= I_n - 2X(X^TX)^{-1}X^T + X(X^TX)^{-1}\mathbf{X^TX}(\underbrace{\mathbf{X^TX}}_{=\mathbf{I_d}})^{-\mathbf{1}}X^T$$

$$= I_n - 2X(X^TX)^{-1}X^T + X(X^TX)^{-1}X^T$$

$$= I_n - X(X^TX)^{-1}X^T = \mathbf{A}$$

Thus : $\mathbf{A^TA = A}$

Step 5 : Conclude

$$E\left[R_n(\hat{\theta})\right] = E_\epsilon\left[\frac{1}{n}||(I_n - X(X^TX)^{-1}X^T)\epsilon||_2^2\right]$$

$$= \frac{\sigma^2}{n}tr(I_n - X(X^TX)^{-1}X^T)$$

$$= \frac{\sigma^2}{n}\left(n - tr(X(X^TX)^{-1}X^T)\right)$$

$$= \frac{\sigma^2}{n}\left(n - tr(X^TX(X^TX)^{-1})\right)$$

$$= \frac{\sigma^2}{n}\left(n - tr(I_d)\right)$$

$$= \frac{\sigma^2}{n}\left(n - d\right)$$

Thus :

$$E[R_X(\hat{\theta})] = E[E[R_n(\hat{\theta})]] = E[\frac{n-d}{n}\sigma^2] = \frac{n-d}{n}\sigma^2$$

Simulation

Step 6

$$E\left[\frac{||y - X\hat{\theta}||_2^2}{n-d}\right]$$

We recognize the fixed design risk with a subtle difference : $\frac{1}{n-d}$ replaced $\frac{1}{n}$, so we can use the formula found in Step 5 and apply this change.

$$= \frac{n-d}{n-d}\sigma^2 = \sigma^2$$

Step 7

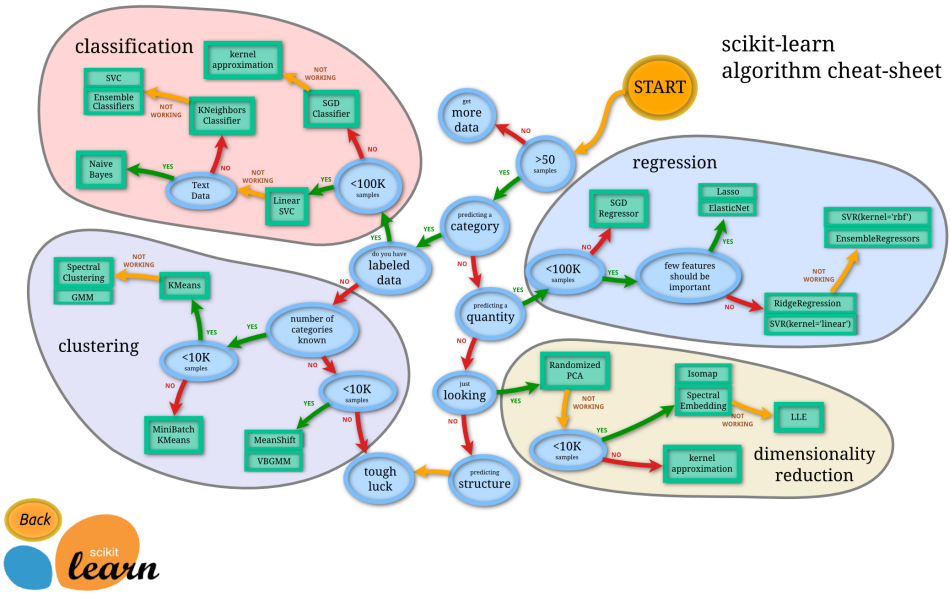
The simulation is in `part3_step7.py`. We suppose :

- n = 10000
- d = 20
- $y = X\theta^*$ with θ^* a random vector

We thus estimate σ^2 with the result of Step 6. With this setting, the simulation estimates a σ^2 of 0, which is an expected result knowing that y is a simple linear function of X without any noise added to it (so the variance of ϵ is 0).
In a second setting, we define y as $y = X\theta^* + \epsilon$ with ϵ being a gaussian vector with a standard deviation of 2 and a mean of 0, for which the simulation estimates σ^2 as 4, thus being still consistent with the theoretical values.

4 Regression

For this section and the next one, we chose `scikit-learn` as our machine learning library because it contains many regression and classification models, it provides easy access to cross validation algorithms and allows us to follow this decision tree :



We should then retrieve the important properties of the dataset :
Number of entries : 1000
Number of features : 20

This needs a regression model that can handle a small set of samples and 20 features

Model	Cross validation score
SVR Linear	0.8920
SVR rbf	0.6820
Ridge alpha=12.0	**0.8932**
Ridge alpha=15.0	**0.8932**
Lasso alpha=12.0	0.8371
RandomForestRegressor	0.8409
AdaBoost Regressor	0.8334
Gradient Boosting Regressor	0.8690

Although we should note that the cross validation score is slightly influenced by the random initialization of the models parameters, the Ridge regression seems to be globally the best regression model in this case.

But to find the best alpha parameter of the Ridge model, we can test different values and evaluate them via their cross validation score usgin the `GridSearchCV` from the scikit-learn modules, from which we can deduce that the best alpha parameter is 60.

5 Classification

As we did in the previous section, we retrieve useful information about the dataset
Number of entries : 1000
Number of features : 20
This needs a classification model that can handle a small set of samples and 20 features. Let's try some of them:

Model	Cross validation score
LinearSVC	**0.886**
KNeighbors	0.856
SVC	0.885
RandomForestClassifier	0.858
AdaBoostClassifier	0.864
GradientBoostingClassifier	0.858

Although we should note that the accuracy is slightly influenced by the random initialization of models parameters, the linear SVC seems to be globally the best

classification model in this case.

We can finally find the best hyperparameters for `LinearSVC` in the same way as in the previous section. This lets us conclude that the best hyperparameters are : `C=1, loss=hinge, penalty=L2` as they get a cross validation score of 0.887 ($+$ 0.1).